Entrapped Polyamines in Biomimetically Synthesized Nanostructured Silica spheres as pH-responsive Gates for Controlled Drug Release



Gousia Begum, ^a M. Vijaya Laxmi^a and Rohit Kumar Rana*^a

Fig. S1 Thermo Gravimetric Analysis (TGA) and corresponding derivative curves of (a) MMS-C-IBU (b) MMS-X and (c) MMS-X-IBU.



Fig. S2 FT-IR spectra of (a) MMS-C and MMS-C-IBU; (b) MMS-X and MMS-X-IBU samples.



Fig. S3 (a) Molecular structure of ibuprofen with atom labeling for the ¹³C NMR assignments; ¹³C MAS NMR spectra of (b) MMS-X-IBU and MMS-X samples. For MMS-X-IBU sample, the peaks from the amino CH_2 of PAH overlap with the peaks from loaded Ibuprofen in the range 10-45 ppm.

Table S1: Line widths of ¹³C signals (δ in ppm) in ibuprofen, MMS-C-IBU and MMS-X-IBU respectively.

Carbon No.	1/2 ^a	3	4 ^b	5	6/7 ^a	8/9 ^a	10	11 ^b	12	13
Ibuprofen	23.4/ 20.3	30.9	44.2	140.5	125.4/ 127.5	129.2/ 130.6	135.6	42.5	15.2	181.5
MMS-C- IBU	21.2	30.3	45.3	141.8	129.7	127.4	137.9	45.2	17.5	179.9
MMS-X- IBU	22.6 (d)	36.9	42.6 (d)	141.7	129.8	121.7	138.9	42.7 (d)	13.4 (d)	183.8

^a[C-1, C-2], [C-6, C-7] & [C-8, C-9] are equivalent carbon atoms (Figure 3b). ^b The signals from C-4 and C-11 overlap.^(d) The signals from PAH overlap with that of ibuprofen in MMS-X-IBU.



Figure S4. Zeta potential plot for (a) MMS-X and (b) MMS-C samples indicating the positive and negative surface charge, respectively.

Table S2: Textural properties of silica samples before and after loading with ibuprofen determined from N_2 - adsorption data.

Sample	$S_{BET}(m^2/g)$	D _{BJH} (nm)	$V_p (mL/g)$
MMS-C	717.67±5	2.695±0.2	0.555±0.1
MMS-X	579.78±8	2.280±0.1	0.528±0.1
MMS-C-IBU	104.73±5	2.318±0.2	0.126±0.04
MMS-X-IBU	87.32±3	1.417 ± 0.4	0.114±0.05